

Benfluralin

1861-40-1 | DTXSID3023899

Model Performance

Model

Data

Weighted KNN model

| 5-fold CV (75%) | | Training (75%) | | Test (25%) | |
|-----------------|------|----------------|------|------------|------|
| Q2 | RMSE | R2 | RMSE | R2 | RMSE |
| 0.91 | 1.08 | 0.91 | 1.08 | 0.92 | 1.00 |

Model Results

Predicted value: 5.29e-05 mmHg

Global applicability domain: Inside

Local applicability domain index: 8.17e-01

Confidence level: 8.15e-01

Nearest Neighbors from the Training Set

| | | |
|---|--|---|
| <div>Image not found</div> <div>Chlorthal-dimethyl</div> <div>Measured: 6.53e-05</div> <div>Predicted: 2.82e-06</div> | <div>Image not found</div> <div>4-Chloro-2-methylphenol</div> <div>Measured: 4.58e-05</div> <div>Predicted: 5.35e-02</div> | <div>Image not found</div> <div>1,2,3,5,7-Pentachloronaphthalene</div> <div>Measured: 8.78e-05</div> <div>Predicted: 2.03e-06</div> |
| <div>Image not found</div> <div>Procymidone</div> <div>Measured: 3.00e-05</div> <div>Predicted: 2.16e-05</div> | <div>Image not found</div> <div>2,3,4,5-Tetrachlorobiphenyl</div> <div>Measured: 3.00e-05</div> <div>Predicted: 1.13e-04</div> | |